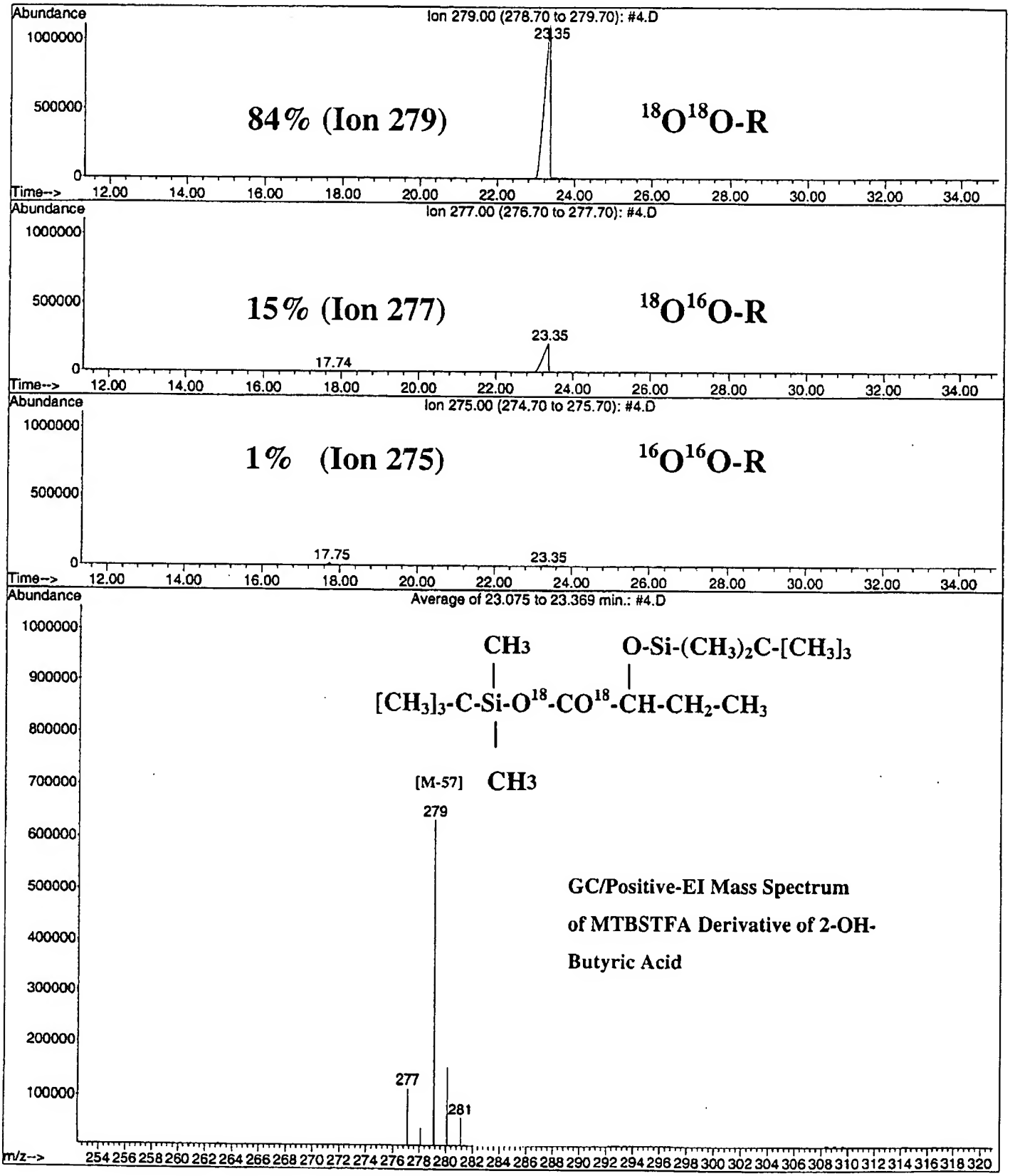
Title: OXYGEN-18 LABELED ORGANIC ACIDS AND USE IN DIAGNOSING METABOLIC DISORDERS
Inventor: Su Chen Atty Dkt. No.: 034827-2601

Figure 1



GC/Positive-EI Mass Spectrum of MTBSTFA Derivative of 2-OH-Butyric Acid

Figure 2

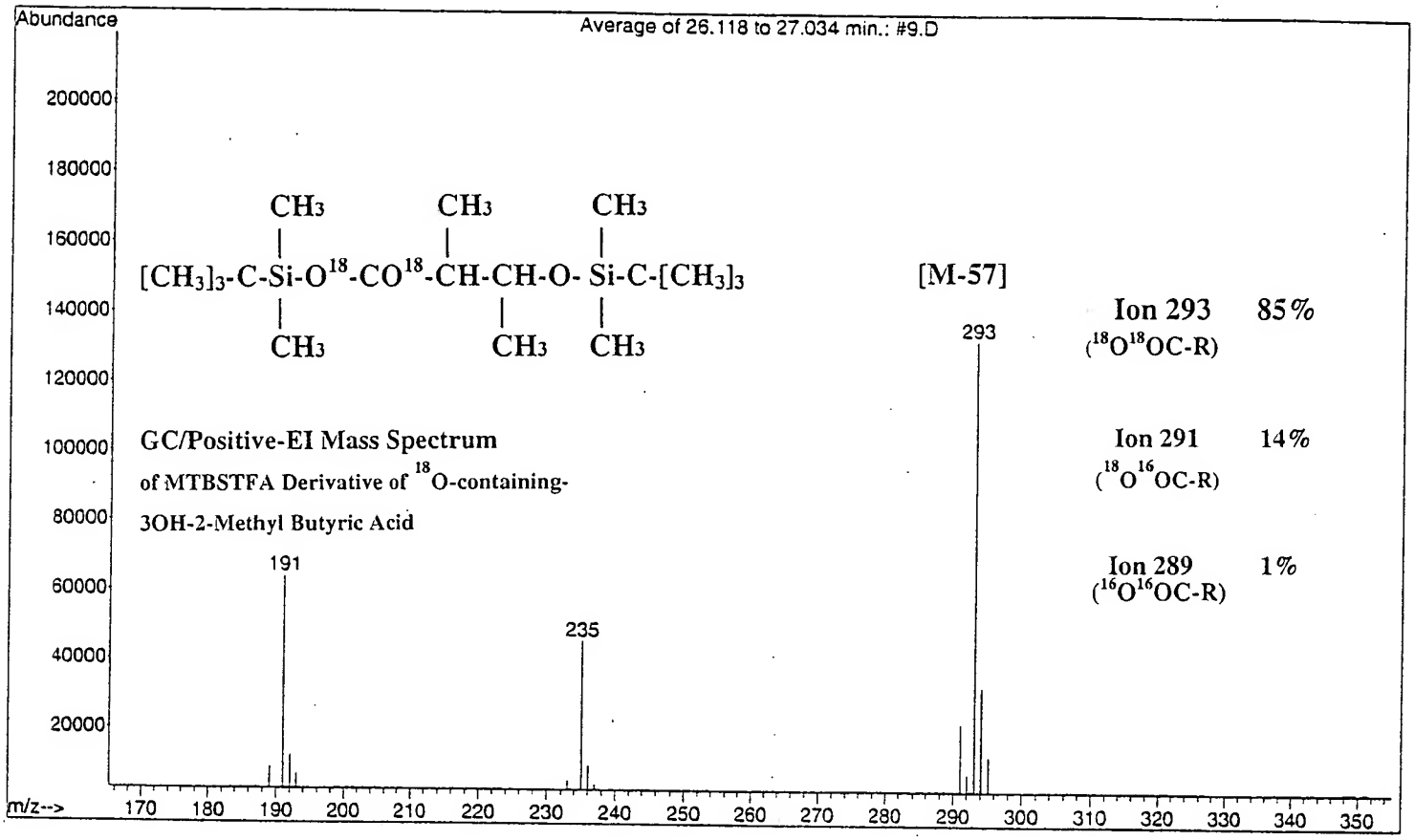
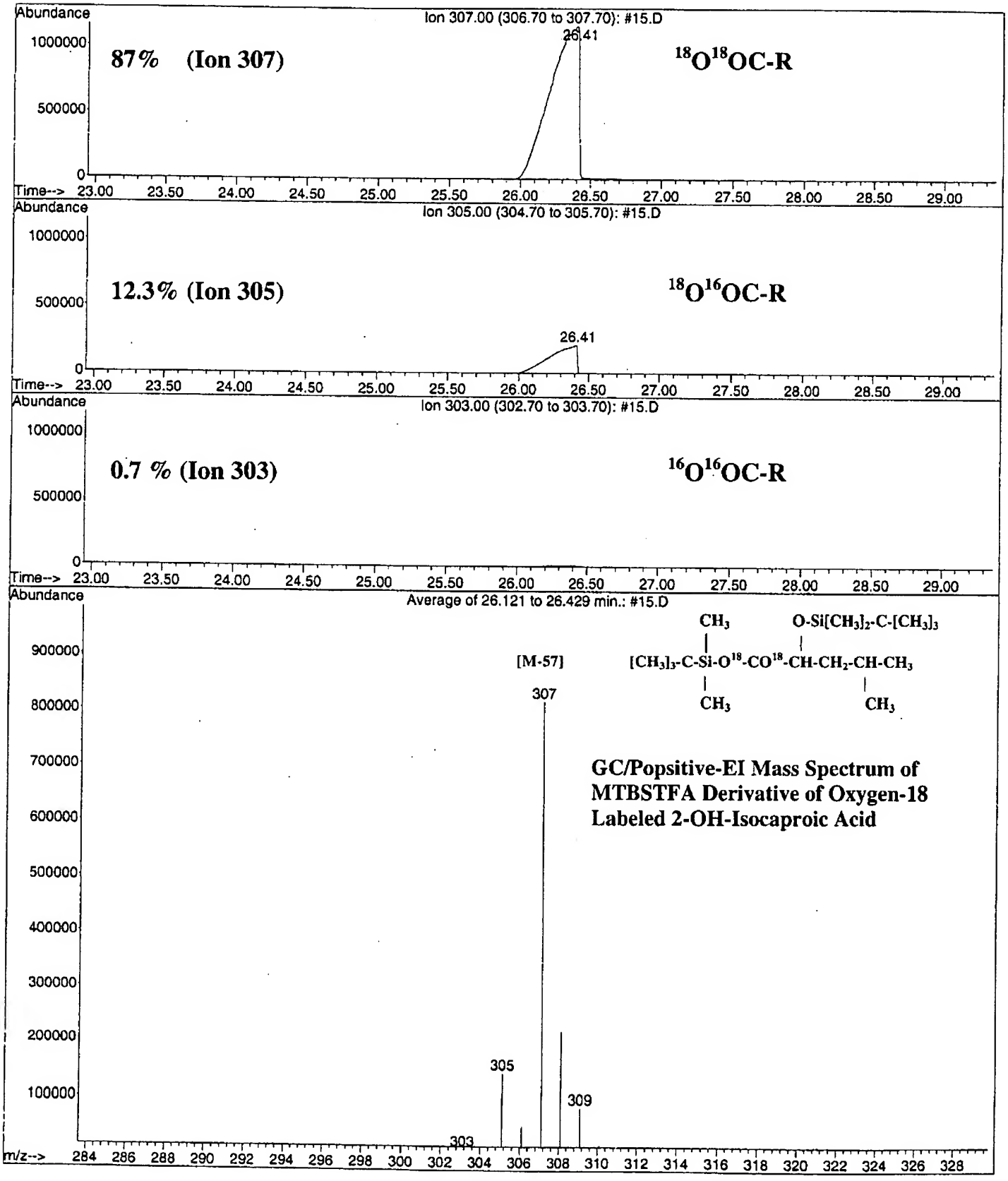

Abundance
Average of 26.118 to 27.034 min.: #9.D
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
CH3 CH3 CH3
[CH3]3-C-Si-O18-CO18-CH-CH-O- Si-C-[CH3]3
CH3 CH3 CH3
[M-57]
293
Ion 293 85%
(18O18OC-R)
Ion 291 14%
(18O16OC-R)
Ion 289 1%
(16O16OC-R)
GC/Positive-EI Mass Spectrum
of MTBSTFA Derivative of 18O-containing-
3OH-2-Methyl Butyric Acid
191
235
m/z-->
170 180 190 200 210 220 230 240 250 260 270 280 290 300 310 320 330 340 350

Figure 3



GC/Popsitive-EI Mass Spectrum of MTBSTFA Derivative of Oxygen-18 Labeled 2-OH-Isocaproic Acid

Figure 4

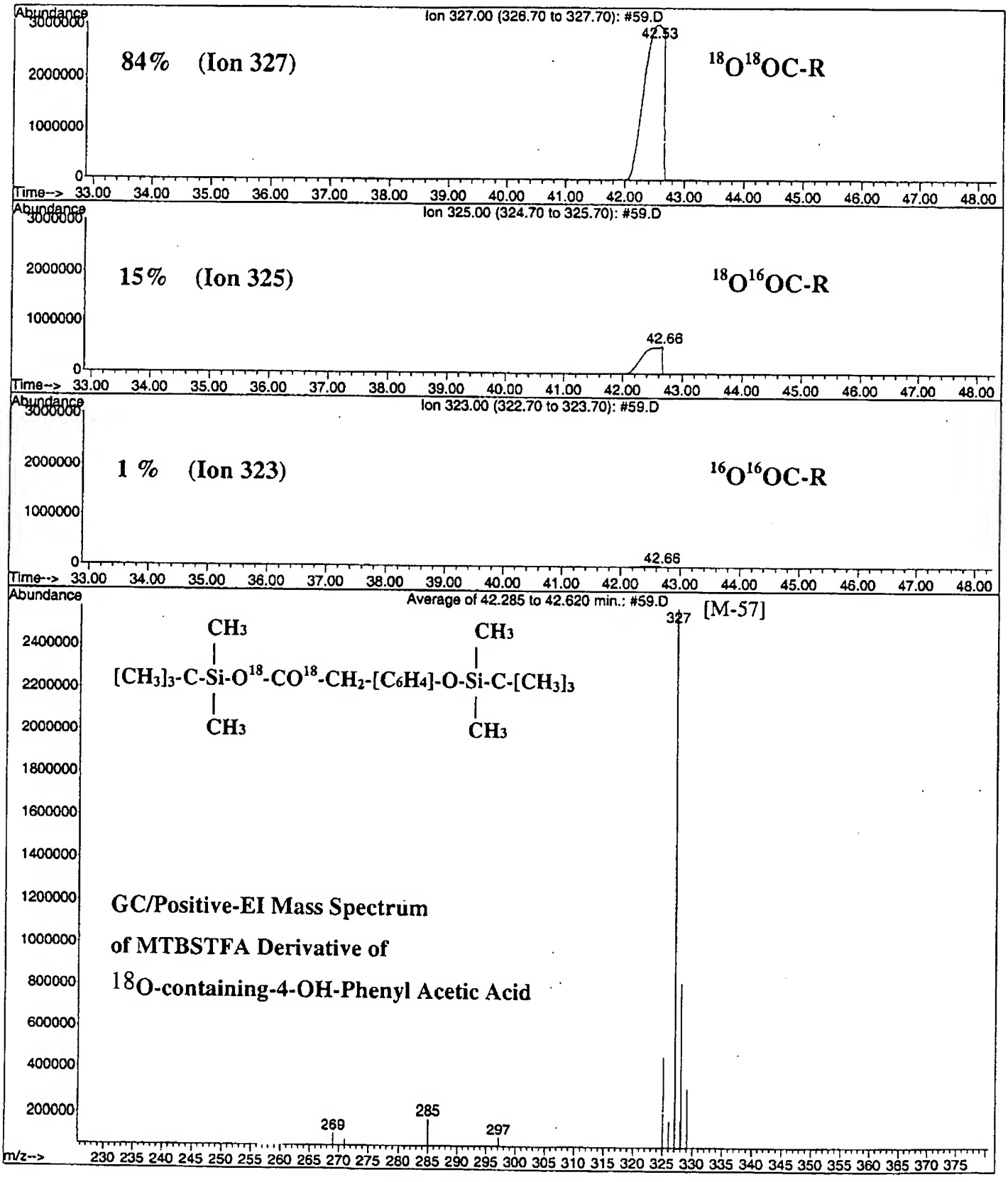

Abundance
Ion 327.00 (326.70 to 327.70): #59.D
42.53
84% (Ion 327)
$^{18}O^{18}OC$-R
Time-->
Abundance
Ion 325.00 (324.70 to 325.70): #59.D
15% (Ion 325)
$^{18}O^{16}OC$-R
42.66
Abundance
Ion 323.00 (322.70 to 323.70): #59.D
1 % (Ion 323)
$^{16}O^{16}OC$-R
42.66
Abundance
Average of 42.285 to 42.620 min.: #59.D
[M-57]
327
[CH3]3-C-Si-O18-CO18-CH2-[C6H4]-O-Si-C-[CH3]3
GC/Positive-EI Mass Spectrum
of MTBSTFA Derivative of
18O-containing-4-OH-Phenyl Acetic Acid
269
285
297
m/z-->

Figure 5

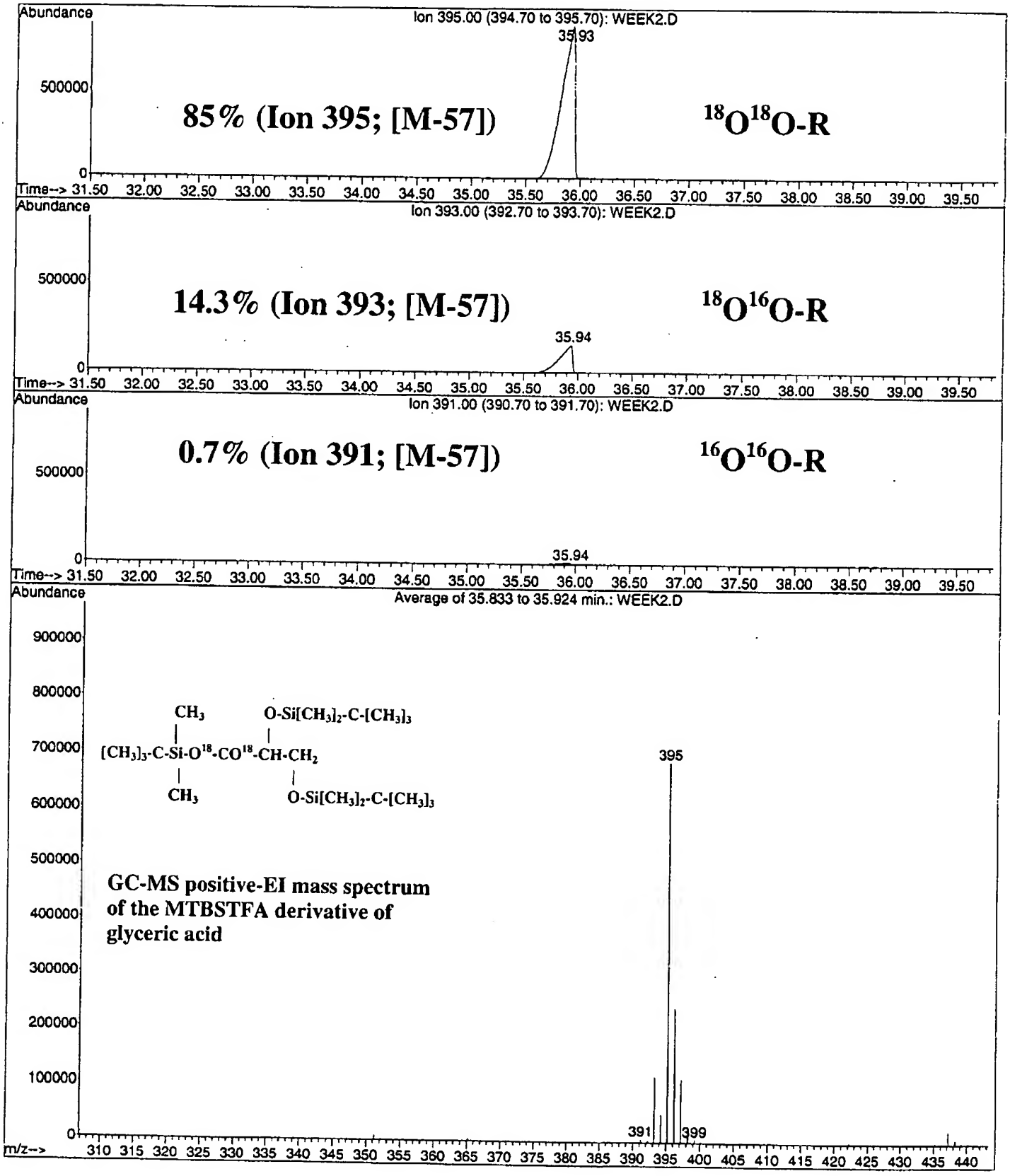

Abundance
Ion 395.00 (394.70 to 395.70): WEEK2.D
35.93
500000
85% (Ion 395; [M-57])
$^{18}O^{18}O$-R
0
Time--> 31.50 32.00 32.50 33.00 33.50 34.00 34.50 35.00 35.50 36.00 36.50 37.00 37.50 38.00 38.50 39.00 39.50
Abundance
Ion 393.00 (392.70 to 393.70): WEEK2.D
500000
14.3% (Ion 393; [M-57])
$^{18}O^{16}O$-R
35.94
0
Time--> 31.50 32.00 32.50 33.00 33.50 34.00 34.50 35.00 35.50 36.00 36.50 37.00 37.50 38.00 38.50 39.00 39.50
Abundance
Ion 391.00 (390.70 to 391.70): WEEK2.D
500000
0.7% (Ion 391; [M-57])
$^{16}O^{16}O$-R
35.94
0
Time--> 31.50 32.00 32.50 33.00 33.50 34.00 34.50 35.00 35.50 36.00 36.50 37.00 37.50 38.00 38.50 39.00 39.50
Abundance
Average of 35.833 to 35.924 min.: WEEK2.D
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
CH3
O-Si[CH3]2-C-[CH3]3
[CH3]3-C-Si-O18-CO18-CH-CH2
CH3
O-Si[CH3]2-C-[CH3]3
GC-MS positive-EI mass spectrum of the MTBSTFA derivative of glyceric acid
395
391
399
m/z-->
310 315 320 325 330 335 340 345 350 355 360 365 370 375 380 385 390 395 400 405 410 415 420 425 430 435 440

Figure 6

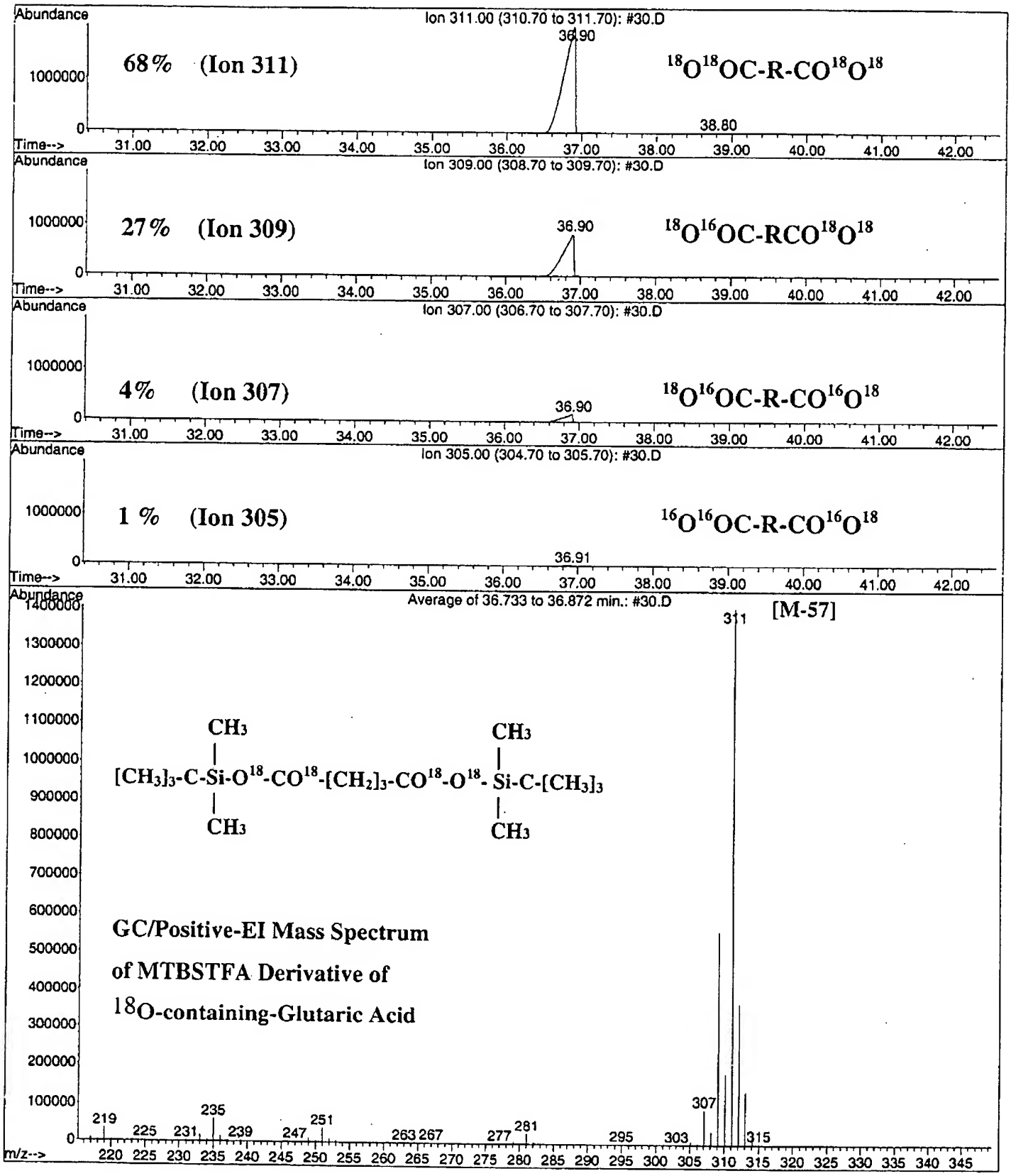

Abundance
Ion 311.00 (310.70 to 311.70): #30.D
68% (Ion 311)
$^{18}O^{18}OC$-R-$CO^{18}O^{18}$
36.90
38.80
Ion 309.00 (308.70 to 309.70): #30.D
27% (Ion 309)
$^{18}O^{16}OC$-R-$CO^{18}O^{18}$
36.90
Ion 307.00 (306.70 to 307.70): #30.D
4% (Ion 307)
$^{18}O^{16}OC$-R-$CO^{16}O^{18}$
36.90
Ion 305.00 (304.70 to 305.70): #30.D
1 % (Ion 305)
$^{16}O^{16}OC$-R-$CO^{16}O^{18}$
36.91
Time-->
Average of 36.733 to 36.872 min.: #30.D
[M-57]
311
$[CH_3]_3$-C-Si-O^{18}-CO^{18}-$[CH_2]_3$-CO^{18}-O^{18}-Si-C-$[CH_3]_3$
GC/Positive-EI Mass Spectrum
of MTBSTFA Derivative of
^{18}O-containing-Glutaric Acid
m/z-->

Figure 7

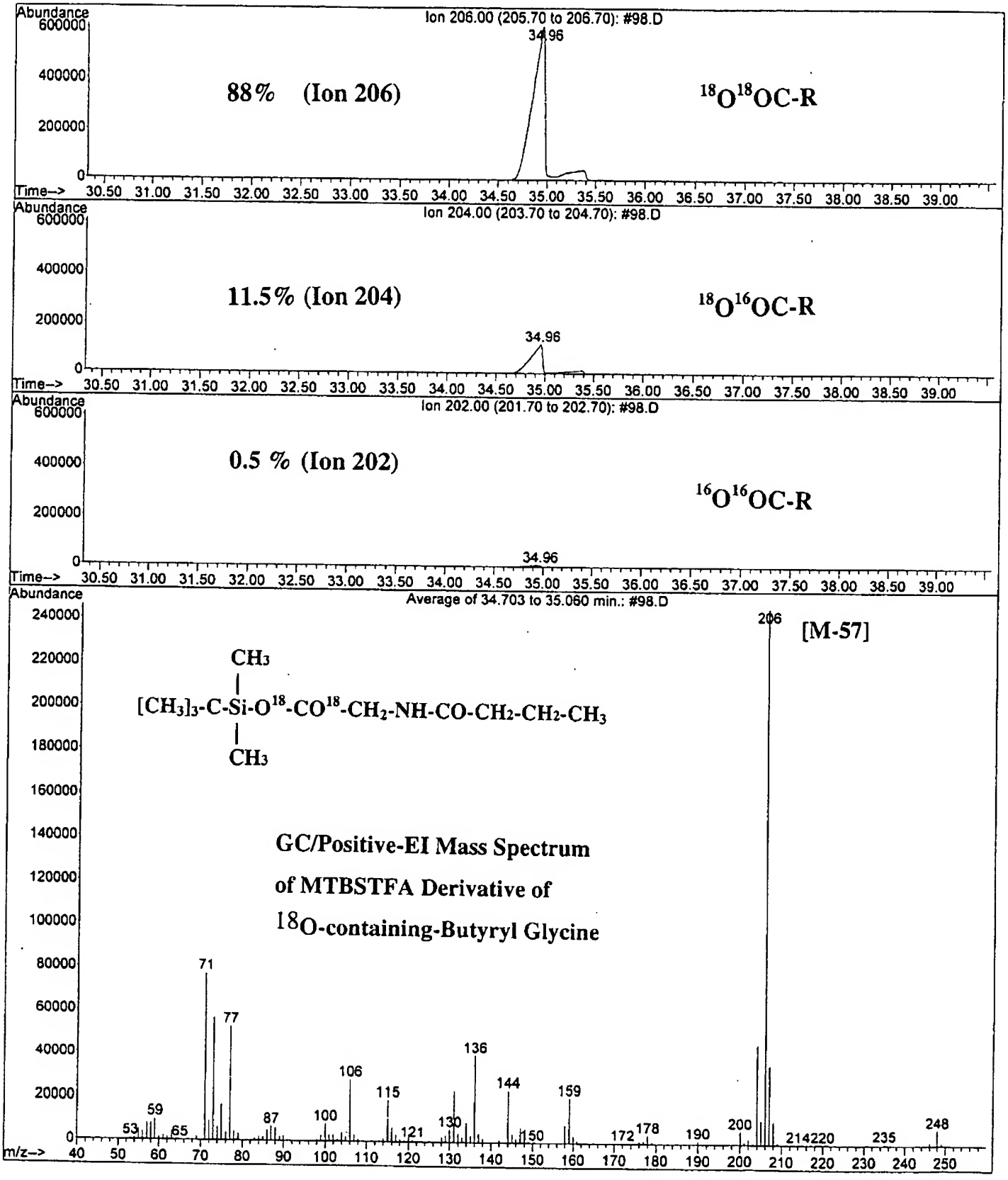

Abundance
Ion 206.00 (205.70 to 206.70): #98.D
34.96
88% (Ion 206)
$^{18}O^{18}OC$-R
Time-->
Abundance
Ion 204.00 (203.70 to 204.70): #98.D
11.5% (Ion 204)
$^{18}O^{16}OC$-R
34.96
Time-->
Abundance
Ion 202.00 (201.70 to 202.70): #98.D
0.5 % (Ion 202)
$^{16}O^{16}OC$-R
34.96
Time-->
Abundance
Average of 34.703 to 35.060 min.: #98.D
206
[M-57]
CH3
[CH3]3-C-Si-O18-CO18-CH2-NH-CO-CH2-CH2-CH3
CH3
GC/Positive-EI Mass Spectrum
of MTBSTFA Derivative of
18O-containing-Butyryl Glycine
m/z-->

Figure 8

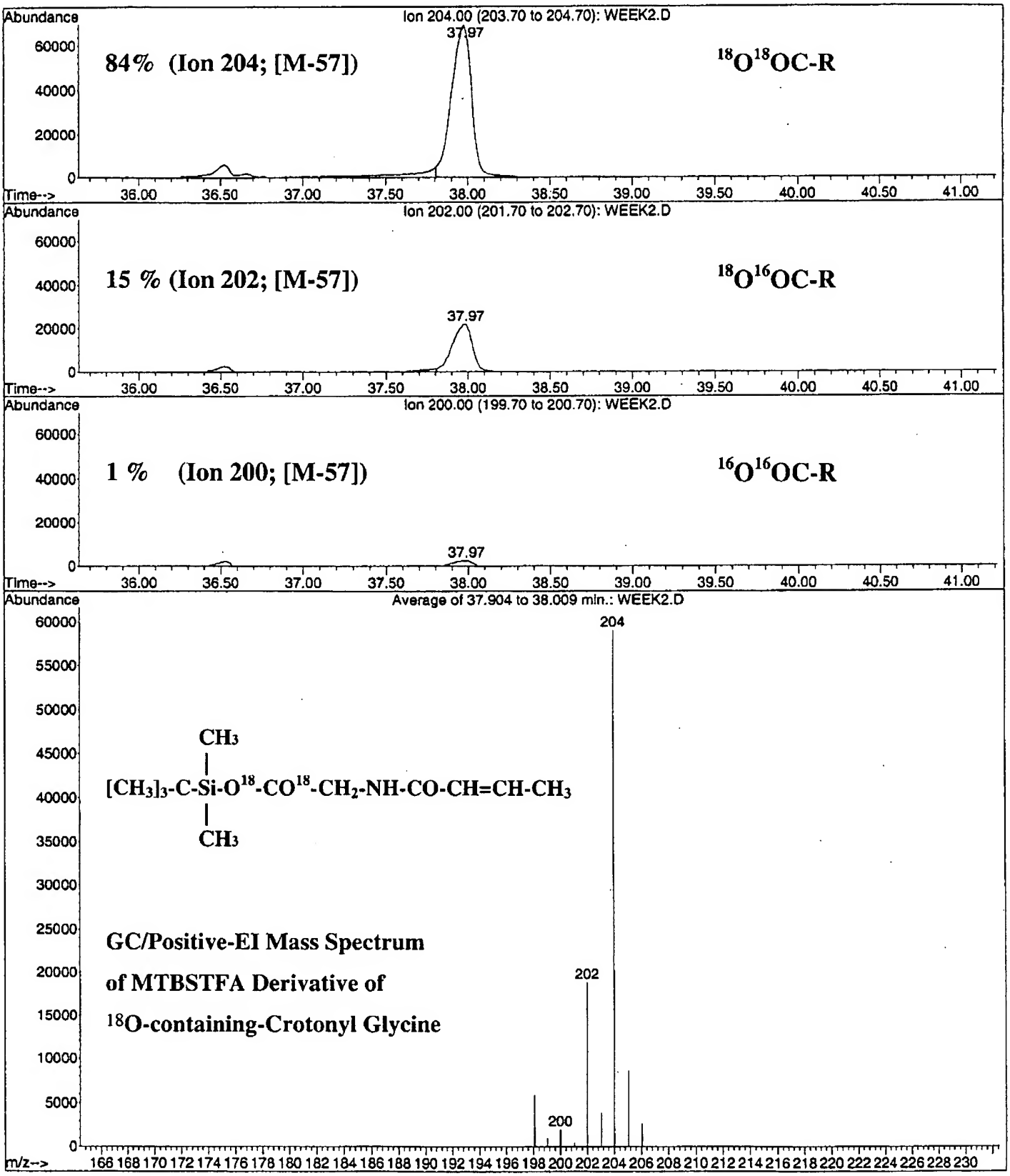

Abundance
Ion 204.00 (203.70 to 204.70): WEEK2.D
37.97
84% (Ion 204; [M-57])
$^{18}O^{18}OC$-R
Time-->
Abundance
Ion 202.00 (201.70 to 202.70): WEEK2.D
15 % (Ion 202; [M-57])
$^{18}O^{16}OC$-R
37.97
Time-->
Abundance
Ion 200.00 (199.70 to 200.70): WEEK2.D
1 % (Ion 200; [M-57])
$^{16}O^{16}OC$-R
37.97
Time-->
Abundance
Average of 37.904 to 38.009 min.: WEEK2.D
204
202
200
$[CH_3]_3$-C-Si-O^{18}-CO^{18}-CH_2-NH-CO-CH=CH-CH_3
GC/Positive-EI Mass Spectrum
of MTBSTFA Derivative of
^{18}O-containing-Crotonyl Glycine
m/z-->

Figure 9

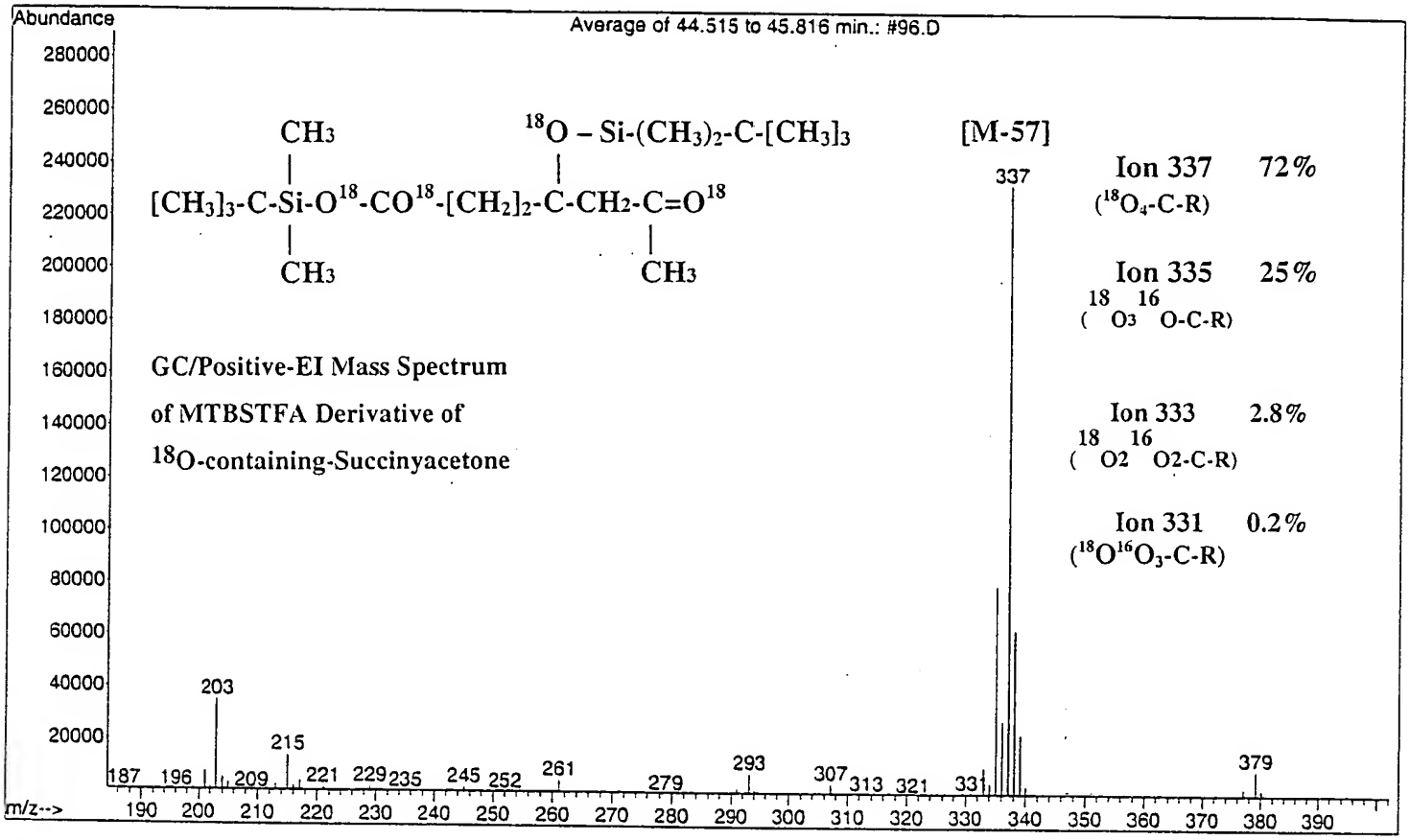
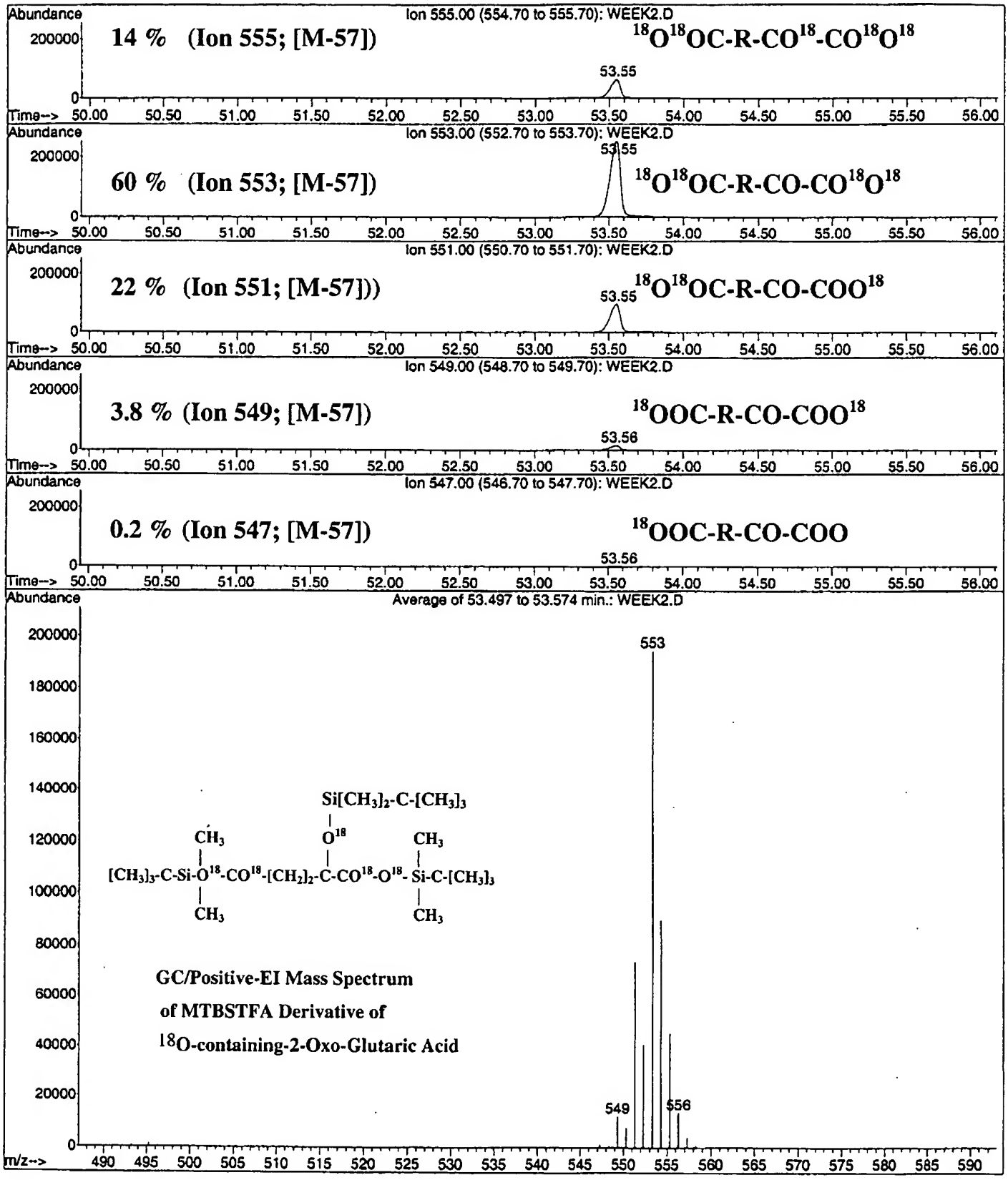

Abundance
Average of 44.515 to 45.816 min.: #96.D
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
CH3
18O – Si-(CH3)2-C-[CH3]3
[M-57]
[CH3]3-C-Si-O18-CO18-[CH2]2-C-CH2-C=O18
CH3
CH3
337
Ion 337 72%
(18O4-C-R)
Ion 335 25%
(18O3 16O-C-R)
Ion 333 2.8%
(18O2 16O2-C-R)
Ion 331 0.2%
(18O16O3-C-R)
GC/Positive-EI Mass Spectrum
of MTBSTFA Derivative of
18O-containing-Succinyacetone
203
215
187 196 209 221 229 235 245 252 261 279 293 307 313 321 331 379
m/z-->
190 200 210 220 230 240 250 260 270 280 290 300 310 320 330 340 350 360 370 380 390

Figure 10



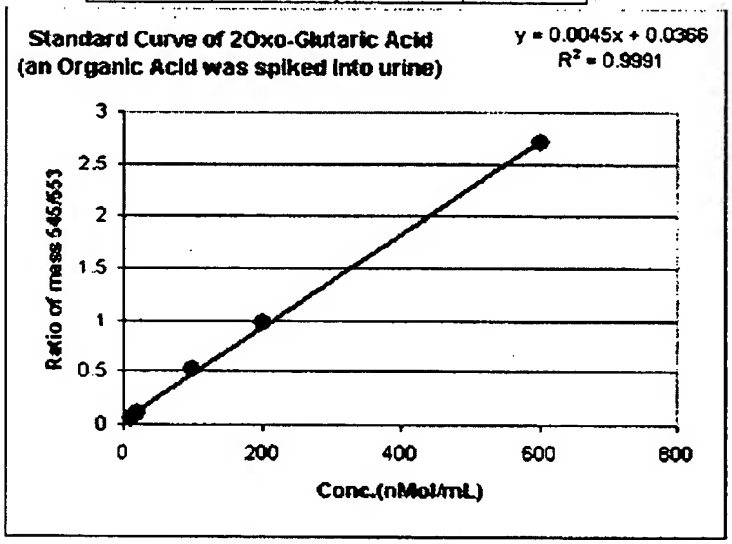
$Si[CH_3]_2$-C-$[CH_3]_3$

$[CH_3]_3$-C-Si-O^{18}-CO^{18}-$[CH_2]_2$-C-CO^{18}-O^{18}-Si-C-$[CH_3]_3$

GC/Positive-EI Mass Spectrum of MTBSTFA Derivative of ^{18}O-containing-2-Oxo-Glutaric Acid

Figure 11. Quantitative Analyses of 2-Oxo Glutaric Acid Using ^{18}O-Standard

nMol/mL	Sta. Area	I.S Area	Ratio
10	99282	1911058	0.051951
20	159741	1548286	0.103173
100	812365	1574774	0.515861
200	1682033	1731756	0.971288
600	6660242	2457755	2.709888



a	b
0.0045	0.0366
0.0045	0.0366
0.0045	0.0366
0.0045	0.0366

	Sam. Area	I.S. Area	x=(y-b)/a (nMol/mL)
QC sample-1 (25 nM)	204106	1522543	**21.65689**
QC sample-2 (500 nM)	4760764	2038057	**510.9628**
Spiked sample-1 (50 nM)	436352	1686953	**49.34729**
Spiked sample-2 (200 nM)	1802739	1848618	**208.5738**

Figure 12

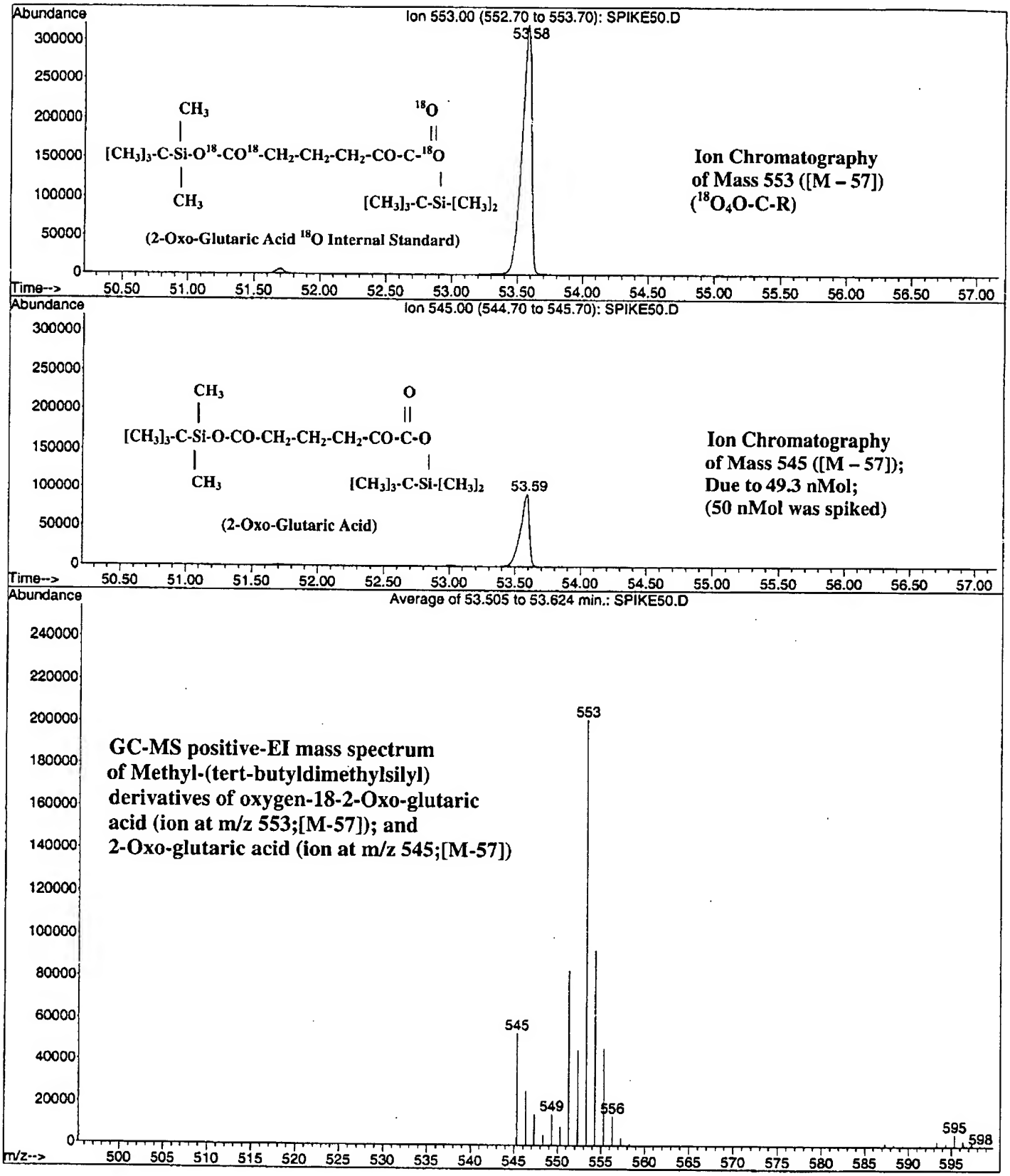
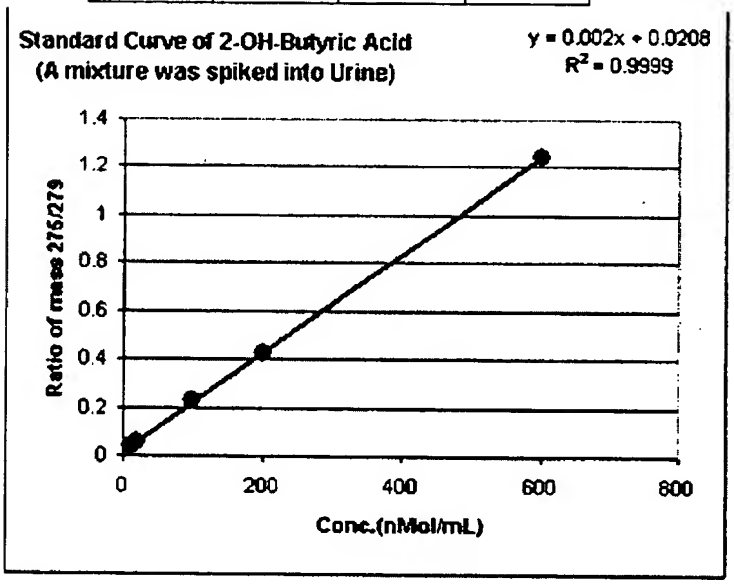

Abundance
Ion 553.00 (552.70 to 553.70): SPIKE50.D
53.58
(2-Oxo-Glutaric Acid ^{18}O Internal Standard)
Ion Chromatography of Mass 553 ([M – 57]) ($^{18}O_4O$-C-R)
Time-->
Abundance
Ion 545.00 (544.70 to 545.70): SPIKE50.D
53.59
(2-Oxo-Glutaric Acid)
Ion Chromatography of Mass 545 ([M – 57]); Due to 49.3 nMol; (50 nMol was spiked)
Time-->
Abundance
Average of 53.505 to 53.624 min.: SPIKE50.D
GC-MS positive-EI mass spectrum of Methyl-(tert-butyldimethylsilyl) derivatives of oxygen-18-2-Oxo-glutaric acid (ion at m/z 553;[M-57]); and 2-Oxo-glutaric acid (ion at m/z 545;[M-57])
553
545
549
556
595
598
m/z-->

Figure 13. Quantitative Analyses of 2-OH-Butyric Acid Using ^{18}O Standard

nMol/mL	Sta. Area	IS. Area	Ratio
10	262735	6538901	0.04018
20	252854	4361156	0.057979
100	1350819	5846408	0.231051
200	2752413	6474802	0.425096
600	7127199	5745837	1.240411



a	b
0.002	0.0208
0.002	0.0208
0.002	0.0208
0.002	0.0208
0.002	0.0208

	Sam. Area	*I.S. Area*	x=(y-b)/a (nMol/mL)
QC sample-1 (25 nM)	455896	5948434	**27.92067**
QC sample-2 (150 nM)	2193354	6626783	**155.0916**
QC sample-3 (500 nM)	5566084	5866775	**463.9734**
Spiked sample-1 (50 nM)	644325	5143162	**52.239**
Spiked sample-2 (400 nM)	5762361	6306218	**446.4793**

Figure 14

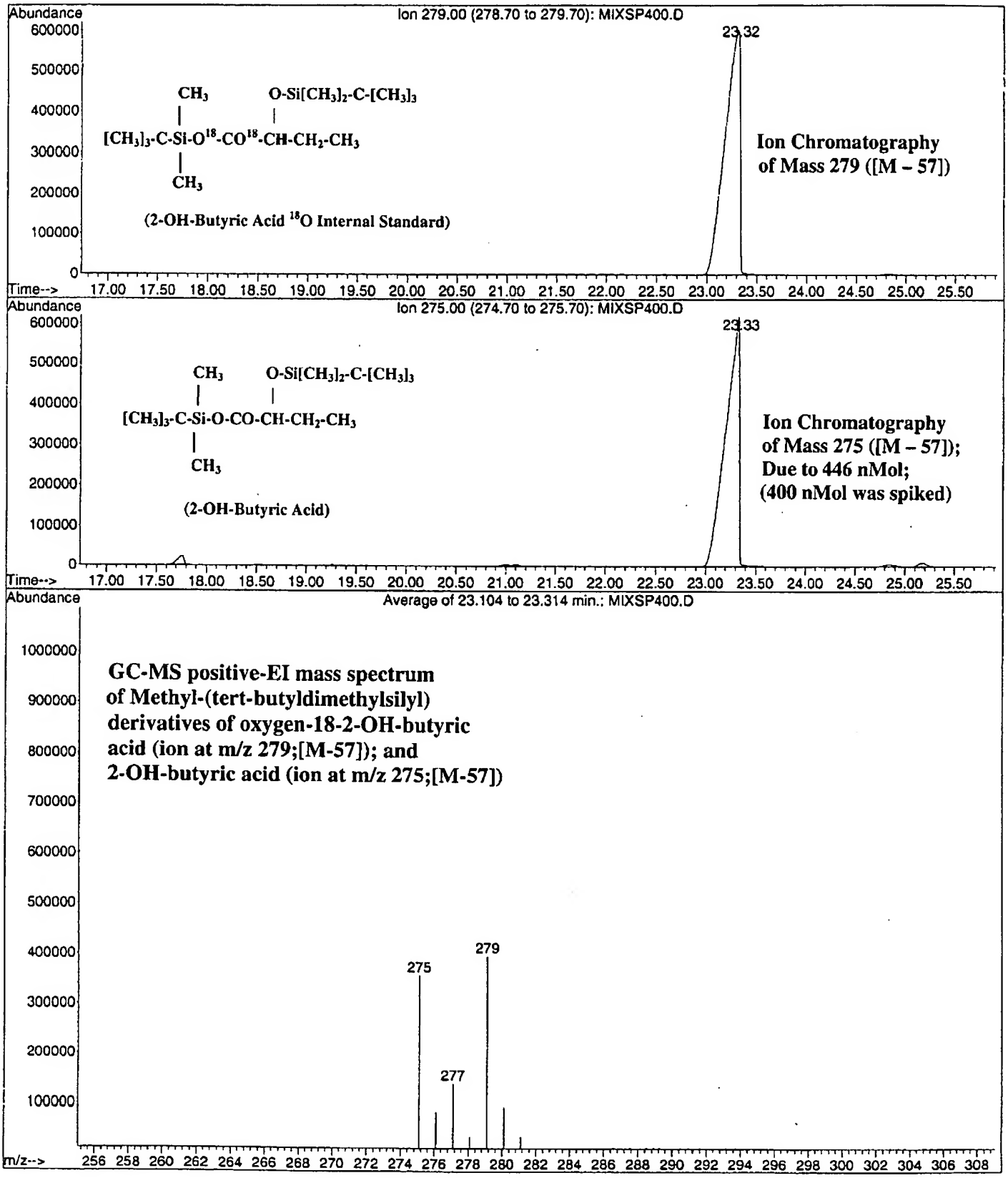
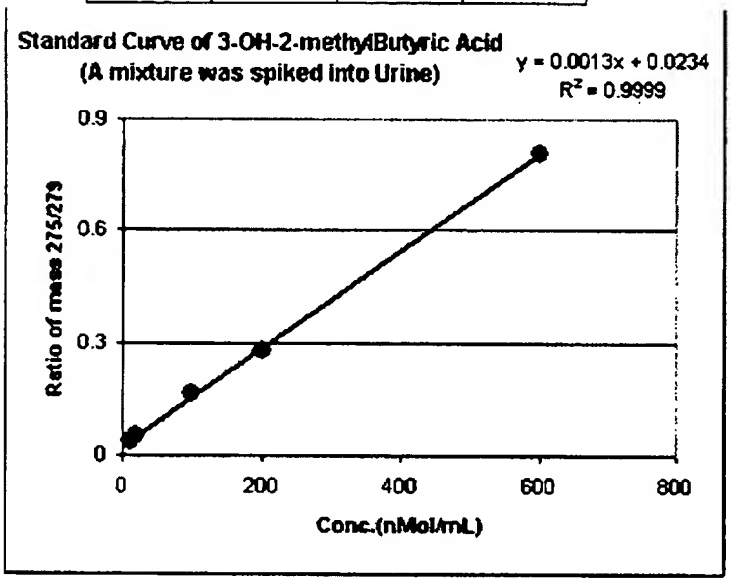

Abundance
Ion 279.00 (278.70 to 279.70): MIXSP400.D
23.32
CH3
O-Si[CH3]2-C-[CH3]3
[CH3]3-C-Si-O18-CO18-CH-CH2-CH3
CH3
(2-OH-Butyric Acid 18O Internal Standard)
Ion Chromatography of Mass 279 ([M – 57])
Time-->
Abundance
Ion 275.00 (274.70 to 275.70): MIXSP400.D
23.33
CH3
O-Si[CH3]2-C-[CH3]3
[CH3]3-C-Si-O-CO-CH-CH2-CH3
CH3
(2-OH-Butyric Acid)
Ion Chromatography of Mass 275 ([M – 57]); Due to 446 nMol; (400 nMol was spiked)
Time-->
Abundance
Average of 23.104 to 23.314 min.: MIXSP400.D
GC-MS positive-EI mass spectrum of Methyl-(tert-butyldimethylsilyl) derivatives of oxygen-18-2-OH-butyric acid (ion at m/z 279;[M-57]); and 2-OH-butyric acid (ion at m/z 275;[M-57])
275
277
279
m/z-->

Figure 15. Quantitative Analyses of 3-OH-3-Methyl Butyric Acid Using ^{18}O-Standard

nMol/mL	Sta. Int.	IS Int.	Ratio
10	4446	121509	0.03659
20	4436	92023	0.048205
100	14663	91820	0.159693
200	28954	103378	0.280079
600	74919	92577	0.809261



a	b
0.0013	0.0234
0.0013	0.0234
0.0013	0.0234
0.0013	0.0234
0.0013	0.0234

	Sam. Int.	I.S. Int.	x=(y-b)/a (nMol/mL)
QC sample-1 (25 nM)	4897	79261	**29.52556**
QC sample-2 (150 nM)	23435	104988	**153.7046**
QC sample-3 (500 nM)	61873	99796	**458.9191**
Spiked sample-1 (50 nM)	9229	101920	**51.65493**
Spiked sample-2 (400 nM)	64894	109735	**436.9001**

Figure 16

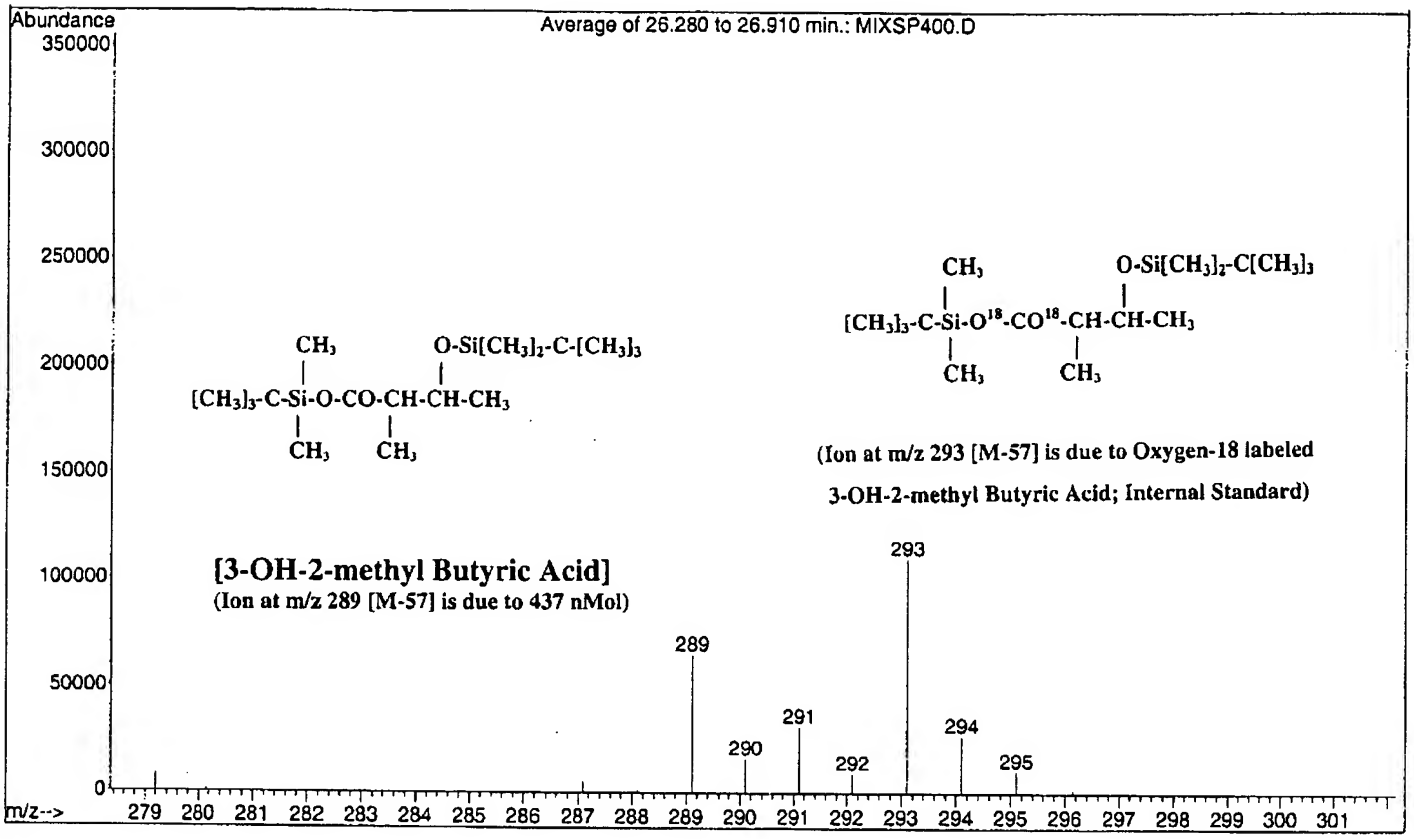
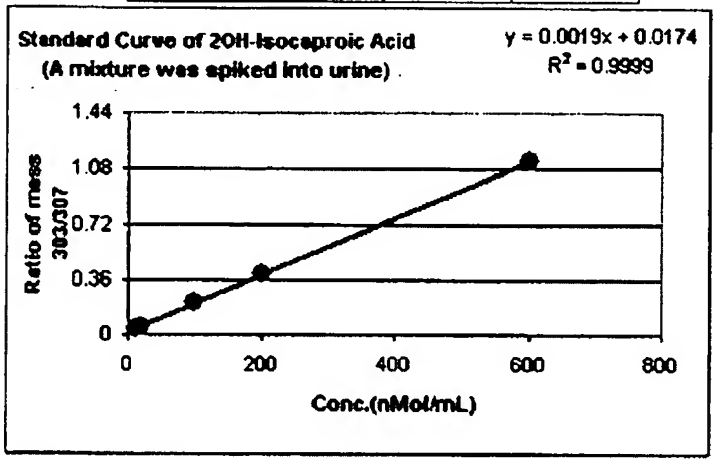

Abundance
Average of 26.280 to 26.910 min.: MIXSP400.D
350000
300000
250000
200000
150000
100000
50000
0
m/z-->
279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300 301
[3-OH-2-methyl Butyric Acid]
(Ion at m/z 289 [M-57] is due to 437 nMol)
(Ion at m/z 293 [M-57] is due to Oxygen-18 labeled
3-OH-2-methyl Butyric Acid; Internal Standard)

Figure 17. Quantitative Analyses of 2-OH-Isocaproic and 5-OH-Hexanoic Acids Using ^{18}O-Standard

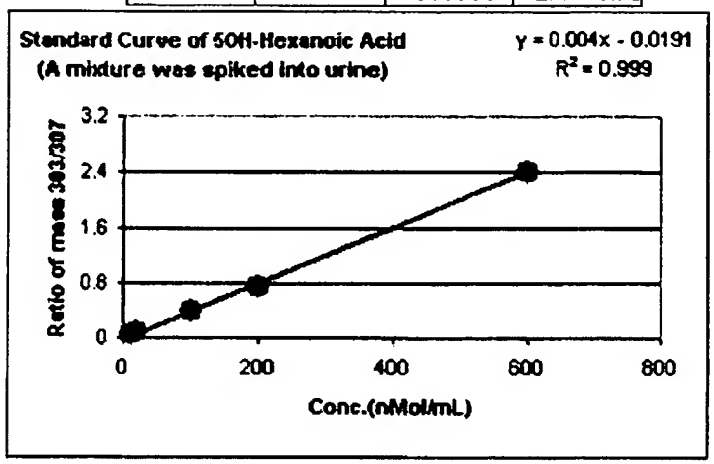
nMol/mL	Sta. Area	IS Area	Ratio
10	433496	13313286	0.032561
20	479074	9358993	0.051189
100	2204397	10582479	0.208306
200	4209784	10736037	0.392117
600	11104139	9830801	1.129525



a	b
0.0019	0.0174
0.0019	0.0174
0.0019	0.0174
0.0019	0.0174
0.0019	0.0174

	Sam. Area	I.S. Area	x=(y-b)/a (nMol/mL)
QC sample-1 (25 nM)	704376	10865259	**24.96225**
QC sample-2 (150 nM)	3500684	11603647	**149.6254**
QC sample-3 (500 nM)	8494331	10369805	**421.9689**
Spiked sample-1 (50 nM)	1150978	10294327	**49.6879**
Spiked sample-2 (400 nM)	9442878	10607592	**459.3684**

nMol/mL	Sta. Area	IS. Area	Ratio
10	556842	13313286	0.041826
20	743576	9358993	0.07945
100	4023905	10582479	0.380242
200	7904895	10736037	0.736295
600	23769123	9830801	2.417822



a	b
0.004	-0.0191
0.004	-0.0191
0.004	-0.0191
0.004	-0.0191
0.004	-0.0191

	Sam. Area	I.S. Area	x=(y-b)/a (nMol/mL)
	1082750	10865259	**29.68812**
	6693634	11603647	**148.989**
	18794712	10369805	**457.8865**
	2070356	10294327	**55.05405**
	18910531	10607592	**450.4589**

Figure 18

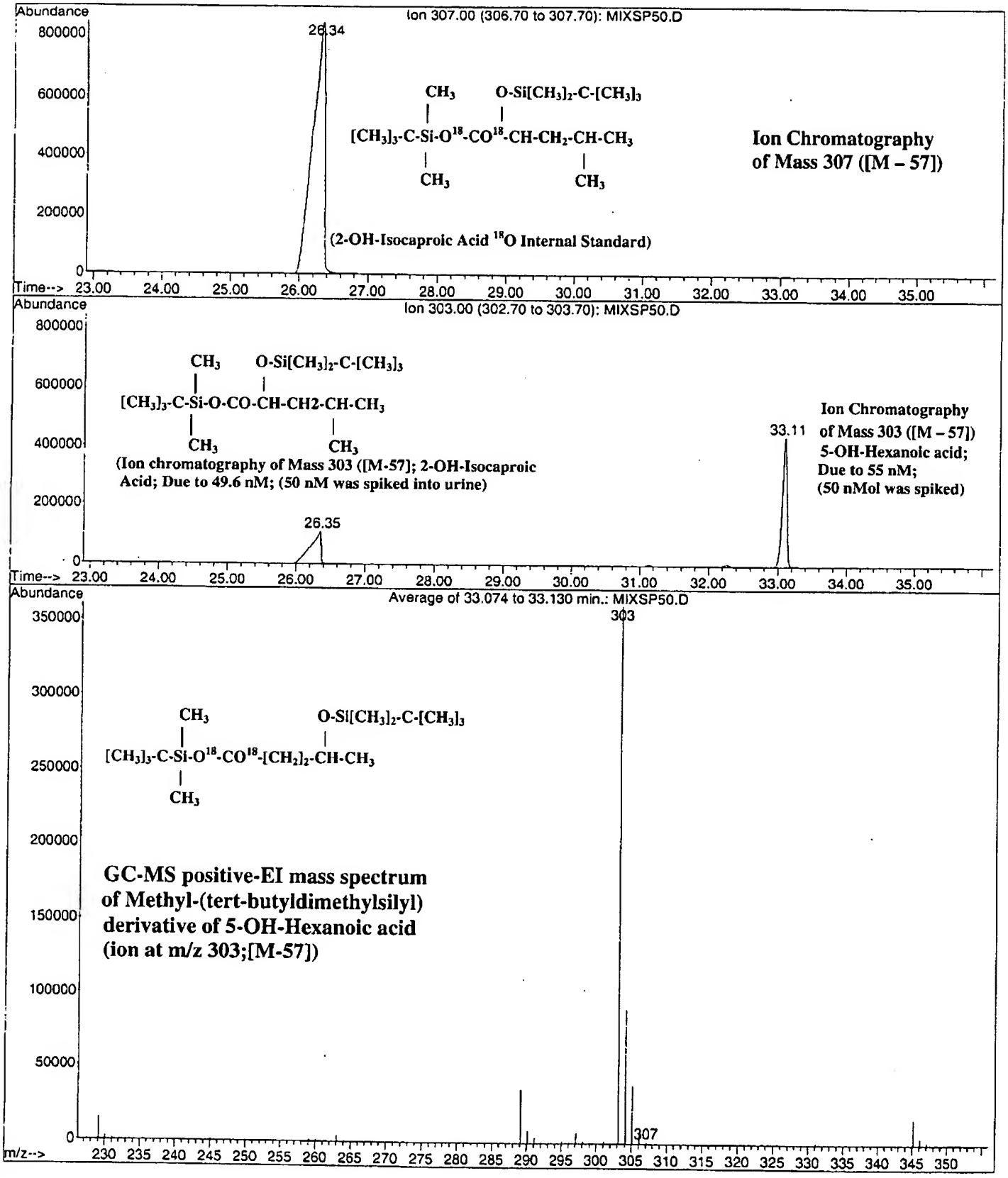
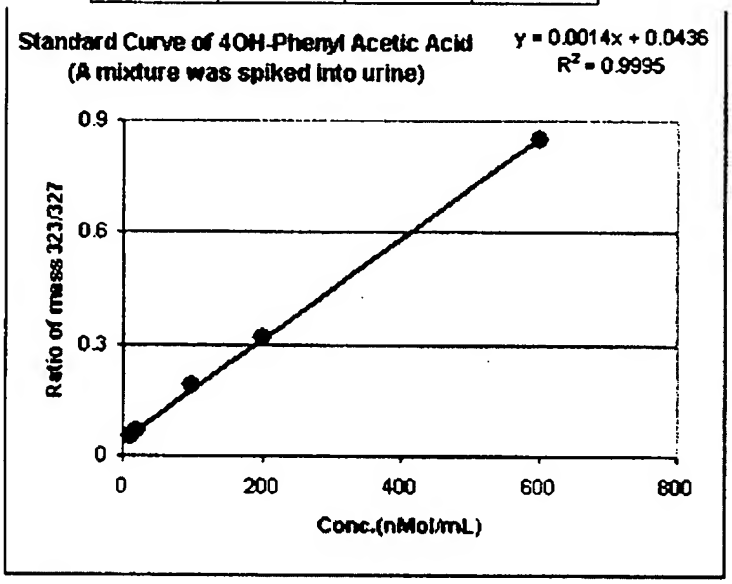

Abundance
Ion 307.00 (306.70 to 307.70): MIXSP50.D
26.34
CH3 O-Si[CH3]2-C-[CH3]3
[CH3]3-C-Si-O18-CO18-CH-CH2-CH-CH3
CH3 CH3
Ion Chromatography of Mass 307 ([M – 57])
(2-OH-Isocaproic Acid 18O Internal Standard)
Time--> 23.00 24.00 25.00 26.00 27.00 28.00 29.00 30.00 31.00 32.00 33.00 34.00 35.00
Abundance
Ion 303.00 (302.70 to 303.70): MIXSP50.D
CH3 O-Si[CH3]2-C-[CH3]3
[CH3]3-C-Si-O-CO-CH-CH2-CH-CH3
CH3 CH3
(Ion chromatography of Mass 303 ([M-57]; 2-OH-Isocaproic Acid; Due to 49.6 nM; (50 nM was spiked into urine)
26.35
33.11
Ion Chromatography of Mass 303 ([M – 57]) 5-OH-Hexanoic acid; Due to 55 nM; (50 nMol was spiked)
Time--> 23.00 24.00 25.00 26.00 27.00 28.00 29.00 30.00 31.00 32.00 33.00 34.00 35.00
Abundance
Average of 33.074 to 33.130 min.: MIXSP50.D
303
CH3 O-Si[CH3]2-C-[CH3]3
[CH3]3-C-Si-O18-CO18-[CH2]2-CH-CH3
CH3
GC-MS positive-EI mass spectrum of Methyl-(tert-butyldimethylsilyl) derivative of 5-OH-Hexanoic acid (ion at m/z 303;[M-57])
307
m/z-->

Figure 19. Quantitative Analyses of 4-OH-Phenyl Acetic Acid Using ^{18}O-Standard

nMol/mL	Sta. Area	IS Area	Ratio
10	3014243	57760161	0.052186
20	2798947	43929289	0.063715
100	8364944	44761329	0.186879
200	14302292	44602241	0.320663
600	36919659	43414038	0.850408



a	b
0.0014	0.0436
0.0014	0.0436
0.0014	0.0436
0.0014	0.0436
0.0014	0.0436

	Sam. Area	*I.S. Area*	x=(y-b)/a (nMol/mL)
QC sample-1 (25 nM)	3364167	45014908	**22.23893**
QC sample-2 (150 nM)	12175131	50417025	**141.3489**
QC sample-2 (500 nM)	28601769	45860639	**414.3336**
Spiked sample-1 (50 nM)	5087964	45749018	**48.29623**
Spiked sample-2 (400 nM)	31012101	45301685	**457.8346**

Figure 20

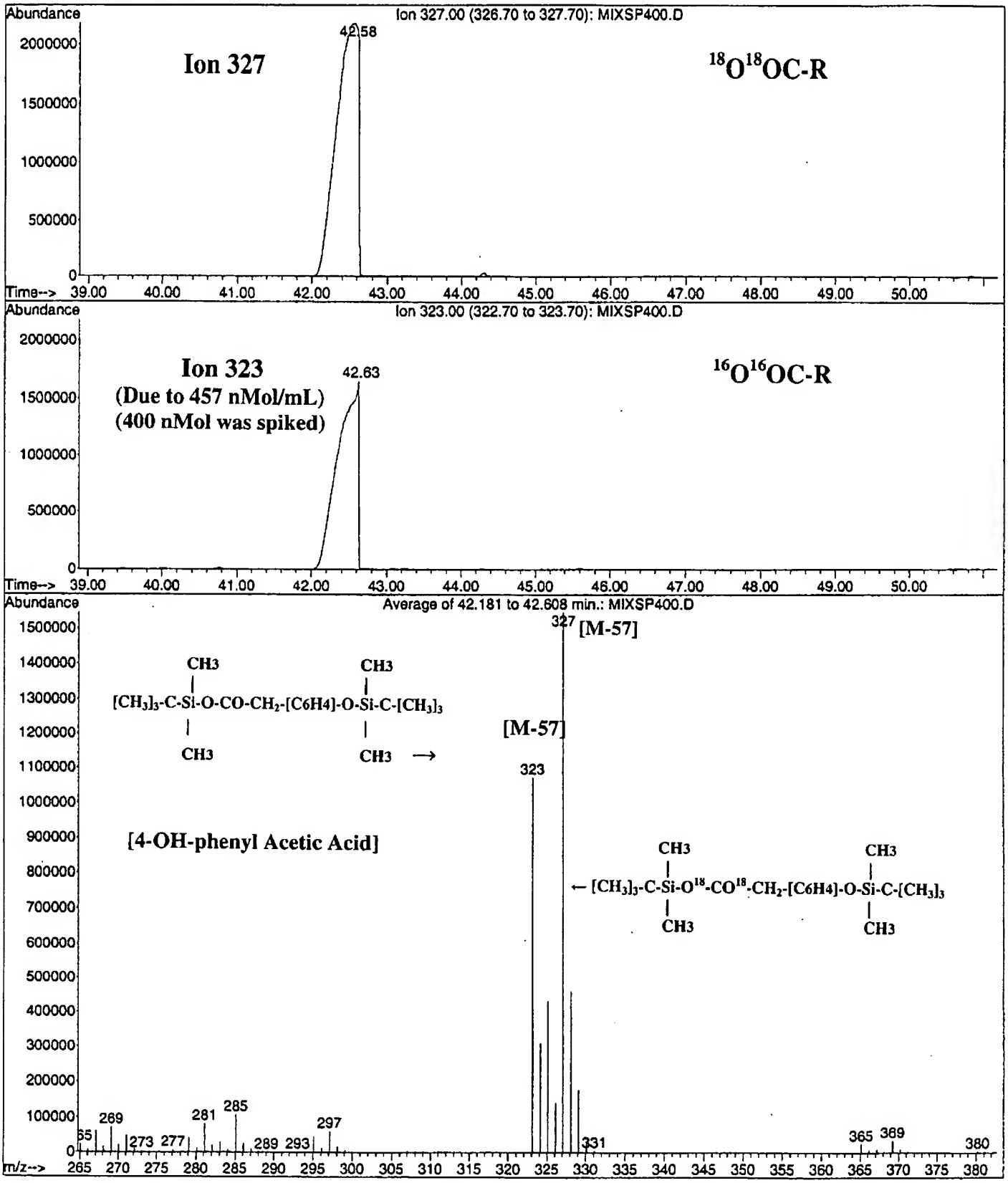
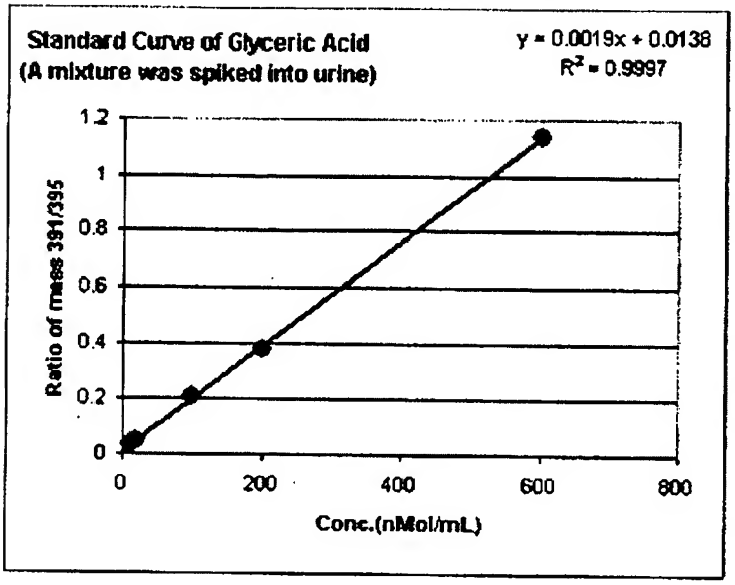

Abundance
Ion 327.00 (326.70 to 327.70): MIXSP400.D
42.58
Ion 327
$^{18}O^{18}OC$-R
Time-->
Abundance
Ion 323.00 (322.70 to 323.70): MIXSP400.D
Ion 323
(Due to 457 nMol/mL)
(400 nMol was spiked)
42.63
$^{16}O^{16}OC$-R
Time-->
Abundance
Average of 42.181 to 42.608 min.: MIXSP400.D
327 [M-57]
[M-57]
323
[4-OH-phenyl Acetic Acid]
m/z-->

Figure 21. Quantitative Analyses of Glyceric Acid Using ^{18}O-Standard

nMol/mL	Sta. Area	IS Area	Ratio
10	26501	801493	0.033065
20	31674	633191	0.050023
100	136532	647351	0.210909
200	256128	680422	0.376425
600	791264	694796	1.138844



a	b
0.0019	0.0138
0.0019	0.0138
0.0019	0.0138
0.0019	0.0138
0.0019	0.0138

	Sam. Area	*I.S. Area*	x=(y-b)/a (nMol/mL)
QC sample-1 (25 nM)	44323	608095	**31.0991**
QC sample-2 (150 nM)	228735	754818	**152.2281**
QC sample-2 (500 nM)	657868	722247	**472.1384**
Spiked sample-1 (50 nM)	74115	669773	**50.97731**
Spiked sample-2 (400 nM)	602067	728922	**427.4574**

Figure 22

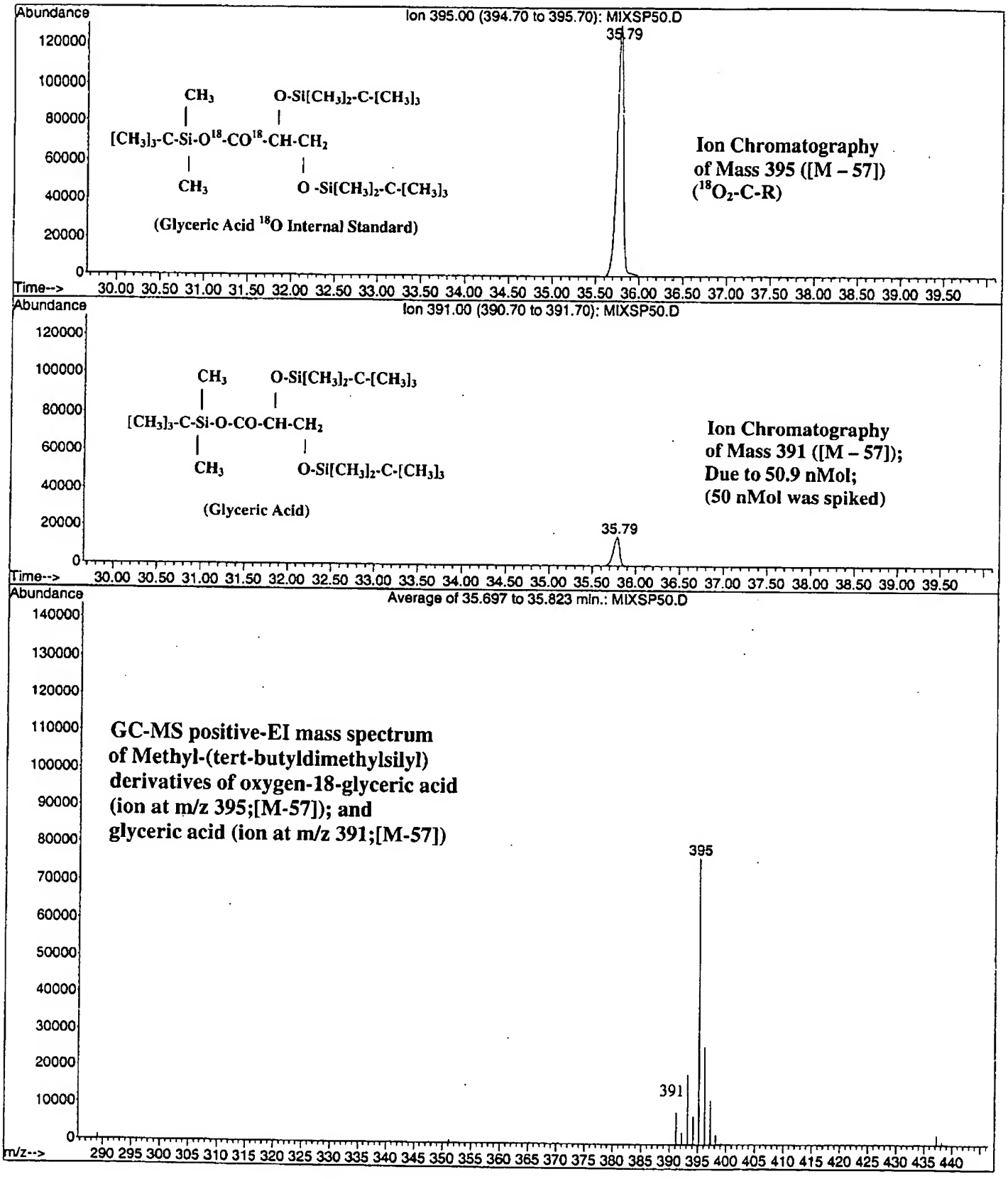
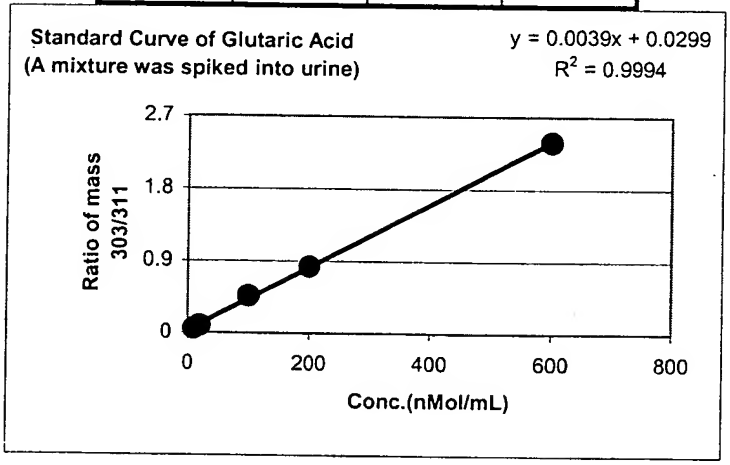

Abundance
Ion 395.00 (394.70 to 395.70): MIXSP50.D
35.79
120000
100000
80000
60000
40000
20000
0
CH3 O-Si[CH3]2-C-[CH3]3
[CH3]3-C-Si-O18-CO18-CH-CH2
CH3 O -Si[CH3]2-C-[CH3]3
(Glyceric Acid 18O Internal Standard)
Ion Chromatography
of Mass 395 ([M – 57])
(18O2-C-R)
Time-->
30.00 30.50 31.00 31.50 32.00 32.50 33.00 33.50 34.00 34.50 35.00 35.50 36.00 36.50 37.00 37.50 38.00 38.50 39.00 39.50
Abundance
Ion 391.00 (390.70 to 391.70): MIXSP50.D
120000
100000
80000
60000
40000
20000
0
CH3 O-Si[CH3]2-C-[CH3]3
[CH3]3-C-Si-O-CO-CH-CH2
CH3 O-Si[CH3]2-C-[CH3]3
(Glyceric Acid)
Ion Chromatography
of Mass 391 ([M – 57]);
Due to 50.9 nMol;
(50 nMol was spiked)
35.79
Time-->
30.00 30.50 31.00 31.50 32.00 32.50 33.00 33.50 34.00 34.50 35.00 35.50 36.00 36.50 37.00 37.50 38.00 38.50 39.00 39.50
Abundance
Average of 35.697 to 35.823 min.: MIXSP50.D
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
GC-MS positive-EI mass spectrum
of Methyl-(tert-butyldimethylsilyl)
derivatives of oxygen-18-glyceric acid
(ion at m/z 395;[M-57]); and
glyceric acid (ion at m/z 391;[M-57])
395
391
m/z-->
290 295 300 305 310 315 320 325 330 335 340 345 350 355 360 365 370 375 380 385 390 395 400 405 410 415 420 425 430 435 440

Figure 23. Quantitative Analyses of Glutaric Acid Using ^{18}O-Standard

nM/mL	Sample	*I.S*	*Ratio*
10	706042	14233824	0.049603
20	957477	10597092	0.090353
100	4807958	10465071	0.459429
200	9209660	11121729	0.828078
600	26198122	10991941	2.383394



a	b
0.0039	0.0299
0.0039	0.0299
0.0039	0.0299
0.0039	0.0299
0.0039	0.0299

	Sam. Area	*I.S. Area*	x=(y-b)/a (nMol/mL)
QC sample-1 (25 nM)	1342471	10520794	**25.05171**
QC sample-2 (150 nM)	7866679	12205842	**157.59**
QC sample-3 (500 nM)	21304159	9350480	**576.5392**
Spiked sample-1 (50 nM)	2518098	11005441	**51.00124**
Spiked sample-2 (400 nM)	16914895	9112873	**468.2702**

Figur 24

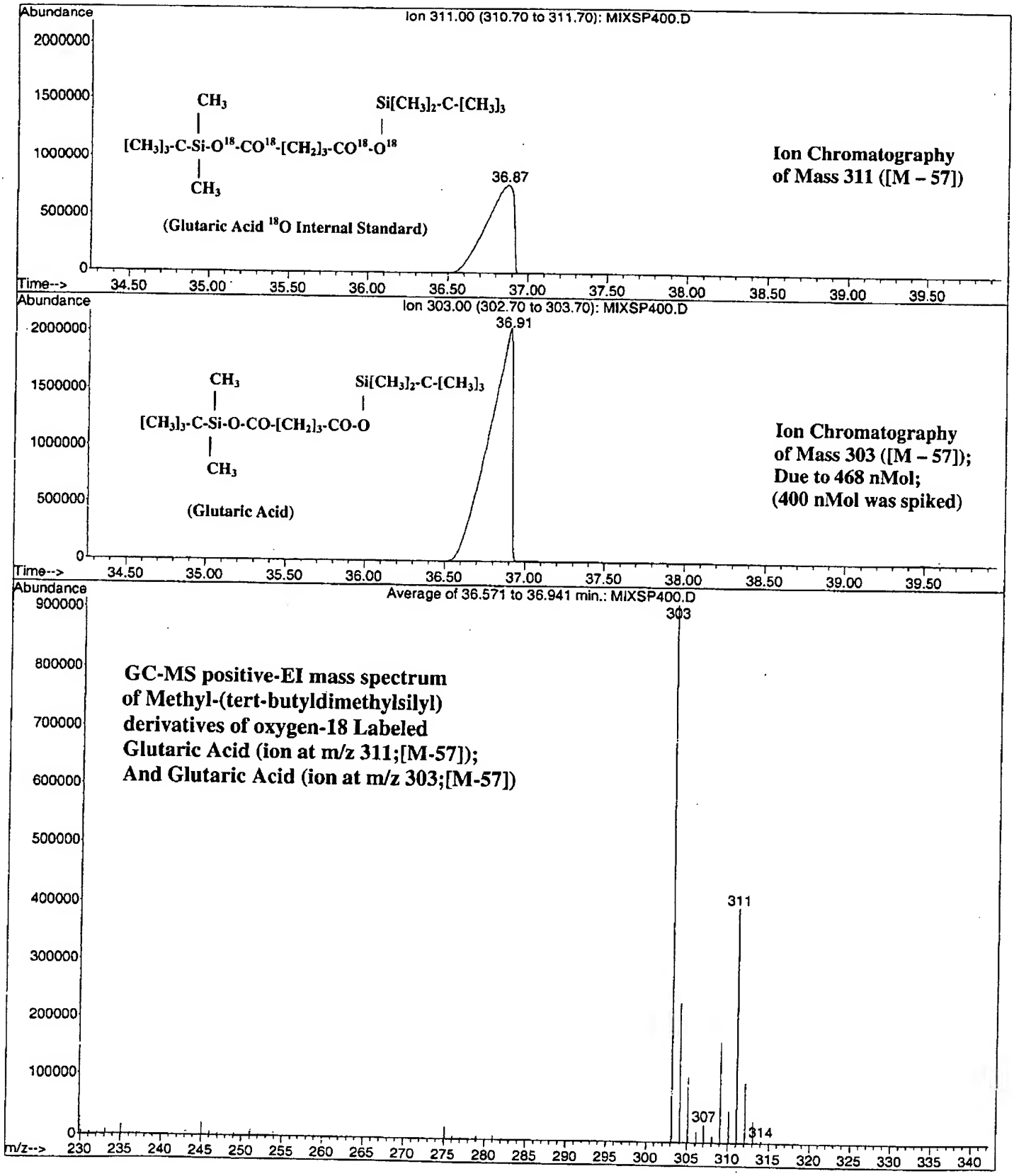
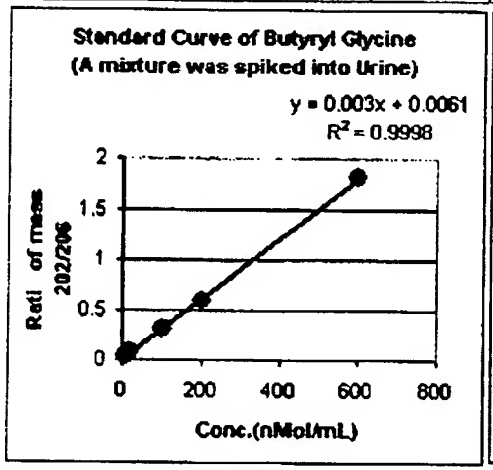

Abundance
Ion 311.00 (310.70 to 311.70): MIXSP400.D
2000000
1500000
1000000
500000
0
CH3
Si[CH3]2-C-[CH3]3
[CH3]3-C-Si-O18-CO18-[CH2]3-CO18-O18
CH3
(Glutaric Acid 18O Internal Standard)
36.87
Ion Chromatography of Mass 311 ([M – 57])
Time-->
34.50 35.00 35.50 36.00 36.50 37.00 37.50 38.00 38.50 39.00 39.50
Abundance
Ion 303.00 (302.70 to 303.70): MIXSP400.D
36.91
2000000
1500000
1000000
500000
0
CH3
Si[CH3]2-C-[CH3]3
[CH3]3-C-Si-O-CO-[CH2]3-CO-O
CH3
(Glutaric Acid)
Ion Chromatography of Mass 303 ([M – 57]); Due to 468 nMol; (400 nMol was spiked)
Time-->
34.50 35.00 35.50 36.00 36.50 37.00 37.50 38.00 38.50 39.00 39.50
Abundance
Average of 36.571 to 36.941 min.: MIXSP400.D
303
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
311
307
314
GC-MS positive-EI mass spectrum of Methyl-(tert-butyldimethylsilyl) derivatives of oxygen-18 Labeled Glutaric Acid (ion at m/z 311;[M-57]); And Glutaric Acid (ion at m/z 303;[M-57])
m/z-->
230 235 240 245 250 255 260 265 270 275 280 285 290 295 300 305 310 315 320 325 330 335 340

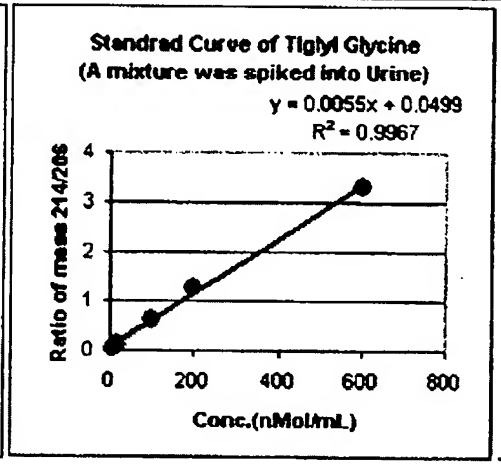
Figure 25. Quantitative Analyses of Butyryl, Tlglyl and Hexanoyl Glycines Using ^{18}O Standard

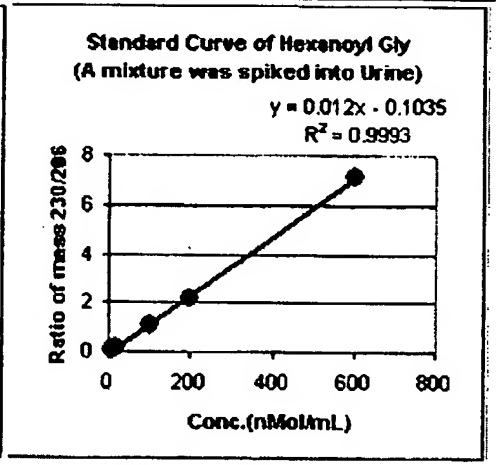
nMol/mL	Sta. Area	IS Area	Ratio
10	148965	3633242	0.041001
20	181515	2692006	0.067427
100	739367	2382535	0.310328
200	1288626	2196672	0.586626
600	3851080	2136479	1.802536

nMol/mL	Sta. Area	IS Area	Ratio
10	195593	3633242	0.053834
20	267010	2692006	0.099186
100	1511459	2382535	0.634391
200	2793427	2196672	1.271663
600	7069631	2136479	3.30901

nMol/mL	Sta. Area	IS Area	Ratio
10	330156	3633242	0.090871
20	451263	2692006	0.167631
100	2535087	2382535	1.064029
200	4792011	2196672	2.181487
600	15246308	2136479	7.136184







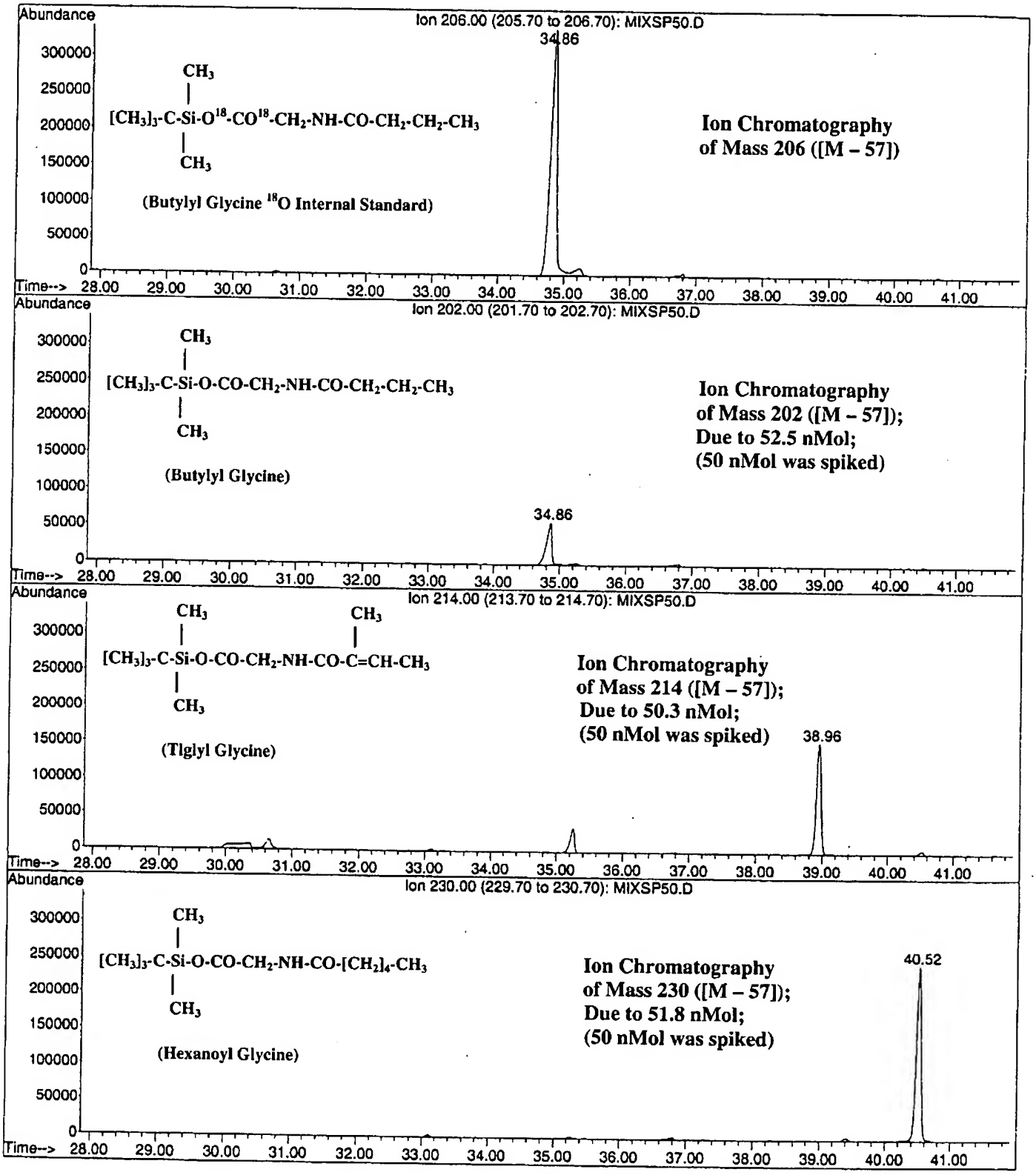
a	b
0.003	0.0061
0.003	0.0061
0.003	0.0061
0.003	0.0061
0.003	0.0061

a	b
0.0055	0.0499
0.0055	0.0499
0.0055	0.0499
0.0055	0.0499
0.0055	0.0499

a	b
0.012	-0.1035
0.012	-0.1035
0.012	-0.1035
0.012	-0.1035
0.012	-0.1035

	Sam. Area	I.S. Area	Results	Sam. Area	I.S. Area	Results	Sam. Area	I.S. Area	Results
QC sample-1 (25 nM)	121537	1237193	**30.71203**	214420	1237193	**22.43849**	264262	1237193	**26.42484**
QC sample-2 (150 nM)	1021922	2196635	**153.0405**	2309002	2196635	**182.0462**	3762059	2196635	**151.3455**
QC sample-3 (500 nM)	2928958	2205317	**440.6782**	5803989	2205317	**469.4393**	11207072	2205317	**432.1118**
Spiked sample-1 (50 nM)	376890	2303216	**52.51214**	751896	2303216	**50.2827**	1193748	2303216	**51.81635**
Spiked sample-2 (400 nM)	2721866	2181828	**413.8054**	5452528	2181828	**445.3026**	11488557	2181828	**447.4221**

Figure 26


Abundance
Ion 206.00 (205.70 to 206.70): MIXSP50.D
34.86
300000
250000
200000
150000
100000
50000
0
CH3
[CH3]3-C-Si-O18-CO18-CH2-NH-CO-CH2-CH2-CH3
CH3
(Butylyl Glycine 18O Internal Standard)
Ion Chromatography
of Mass 206 ([M – 57])
Time--> 28.00 29.00 30.00 31.00 32.00 33.00 34.00 35.00 36.00 37.00 38.00 39.00 40.00 41.00
Abundance
Ion 202.00 (201.70 to 202.70): MIXSP50.D
CH3
[CH3]3-C-Si-O-CO-CH2-NH-CO-CH2-CH2-CH3
CH3
(Butylyl Glycine)
Ion Chromatography
of Mass 202 ([M – 57]);
Due to 52.5 nMol;
(50 nMol was spiked)
34.86
Time--> 28.00 29.00 30.00 31.00 32.00 33.00 34.00 35.00 36.00 37.00 38.00 39.00 40.00 41.00
Abundance
Ion 214.00 (213.70 to 214.70): MIXSP50.D
CH3
CH3
[CH3]3-C-Si-O-CO-CH2-NH-CO-C=CH-CH3
CH3
(Tlglyl Glycine)
Ion Chromatography
of Mass 214 ([M – 57]);
Due to 50.3 nMol;
(50 nMol was spiked)
38.96
Time--> 28.00 29.00 30.00 31.00 32.00 33.00 34.00 35.00 36.00 37.00 38.00 39.00 40.00 41.00
Abundance
Ion 230.00 (229.70 to 230.70): MIXSP50.D
CH3
[CH3]3-C-Si-O-CO-CH2-NH-CO-[CH2]4-CH3
CH3
(Hexanoyl Glycine)
Ion Chromatography
of Mass 230 ([M – 57]);
Due to 51.8 nMol;
(50 nMol was spiked)
40.52
Time--> 28.00 29.00 30.00 31.00 32.00 33.00 34.00 35.00 36.00 37.00 38.00 39.00 40.00 41.00